

# Magnetic properties and concurrence for fluid $^3\text{He}$ on kagome lattice

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## Abstract

We present the results of magnetic properties and entanglement for kagome lattice using Heisenberg model with two-, and three-site exchange interactions in strong magnetic field. Kagome lattice correspond to the third layer of fluid  $^3\text{He}$  absorbed on the surface of graphite. The magnetic properties and concurrence as a measure of pairwise thermal entanglement are studied by means of variational mean-field like treatment based on Gibbs-Bogoliubov inequality. The system exhibits different magnetic behaviors, depending on the values of the exchange parameters ( $J_2, J_3$ ). We have obtained the magnetization plateaus at low temperatures. The central theme of the paper is the comparing the entanglement and magnetic behavior for kagome lattice. We have found that in the antiferromagnetic region behaviour of the concurrence coincides with the magnetization one.

## 1 Introduction

One can model solid and fluid  $^3\text{He}$  films as the systems of almost localized identical fermions. Since the light mass spin-1/2  $^3\text{He}$  atoms are subject to a weak attractive potential, the theoretical explanation of magnetism is based on the multiple-spin exchange mechanism [1]. An important case is represented by solid and fluid  $^3\text{He}$  films absorbed on the surface of graphite [2, 3, 4] since it is a typical example of a two-dimensional frustrated quantum-spin system [5]. The first and second layers of the system form a triangular lattice [6], while the third one forms a system of quantum 1/2 spins on a kagome lattice [7].

The phenomenon of magnetization plateau has been studied during the past decade both experimentally and theoretically. The plateaus may be exhibited in the magnetization curves of quantum spin systems at very low temperatures in case of

strong external field. Magnetization plateaus appear in a wide range of models on chains, ladders, hierarchical lattices, theoretically analysed by dynamical, transfer matrix approaches and exact diagonalization in clusters (see Ref. [8]-[18]). In [19] dynamical system theory has been used to study magnetization plateaus on the kagome chain with two-, three- and six-site exchange interactions.

Recent years much effort has been put into studying the entanglement of multipartite systems both qualitatively and quantitatively [20, 21]. Entanglement has gained renewed interest with the development of quantum information science. Entangled states constitute a valuable resource in quantum information processing [22]. Numerous different methods of entanglement measuring have been proposed for its quantification [23]. In this paper we use concurrence [24] as entanglement measure of the spin-1/2 system.

In the present paper mean-field like approach, based on the Gibbs-Bogoliubov inequality, was used to study entanglement and magnetic properties of a kagome lattice [25]. This method can also be applied to study thermal entanglement in many-body systems [26, 27].

The key result of the paper is concentrated on the comparison of specific (peaks and plateaus) features in magnetization and thermal entanglement properties in the above mentioned model using variational mean-field like Gibbs-Bogoliubov inequality.

This paper is organized as follows: in Section 2 we introduce the Heisenberg model on the kagome lattice with two- and three-site exchange interactions. In Section 3 mean-field like approximation, based on Gibbs-Bogoliubov inequality, has applied on kagome lattice. The magnetic properties of the model are investigated in Section 4. In Section 5 concurrence as a measure of entanglement is studied and compared with magnetic properties of kagome lattice. The conclusive remarks are given in Sec. 6.

## 2 Heisenberg model Hamiltonian on kagome lattice with two-, and three-site exchanges interactions

The Hamiltonian of the Heisenberg model is

$$H = H_{ex} + H_Z, \quad (1)$$

where  $H_{ex}$  represent spin exchanges and  $H_Z$  is responsible for magnetism. The expression for  $H_Z$  can be written as

$$H_Z = - \sum_i \frac{\gamma}{2} \hbar \mathbf{B} \boldsymbol{\sigma}_i \equiv -\hbar \sum_i \sigma_i^z, \quad (2)$$

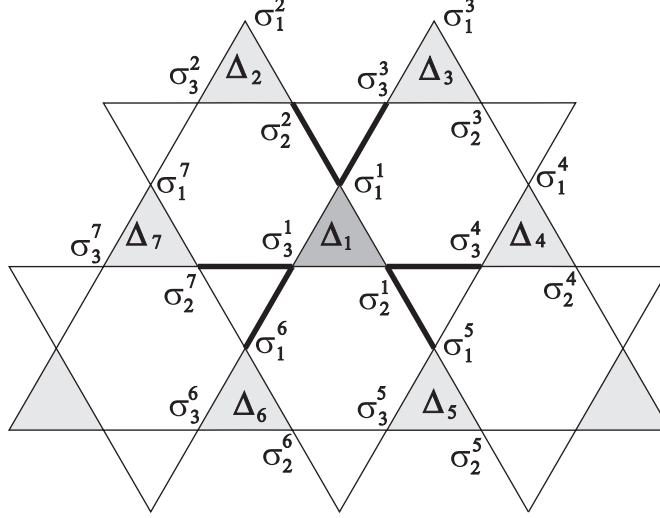


Figure 1: Kagome lattice.

where  $\gamma, \mathbf{B}$  are gyromagnetic ratio and magnetic field. According to [1] the multiple spin exchanges Hamiltonian can be written as

$$H_{ex} = J_2 \sum_{\langle i,j \rangle} P_{i,j} - J_3 \sum_{\langle i,j,k \rangle} (P_{i,j,k} + P_{i,j,k}^{-1}) + \dots, \quad (3)$$

where  $P_{i,j}, P_{i,j,k}$  represent the two-, and three-spin cyclic permutation operators. The sums are taken over all distinct two- and three-cycles. The expression of pair transposition operator  $P_{ij}$  has been given by Dirac

$$P_{i,j} = \frac{1}{2} (1 + \boldsymbol{\sigma}_i \boldsymbol{\sigma}_j), \quad (4)$$

where  $\boldsymbol{\sigma}_i$  are the Pauli matrixes, acting on the spin at the  $i$ -th site. Using this expression for  $P_{i,k}$  one can find the expressions for the other operators of cyclic rearrangement, (see [1, 16]) Here is the expression for three spin exchange operator:

$$P_{i,j,k} + P_{i,j,k}^{-1} = \frac{1}{2} (1 + \boldsymbol{\sigma}_i \boldsymbol{\sigma}_j + \boldsymbol{\sigma}_j \boldsymbol{\sigma}_k + \boldsymbol{\sigma}_k \boldsymbol{\sigma}_i). \quad (5)$$

As mentioned above the third layer of  ${}^3He$  system is kagome lattice (see Fig 1). In kagome lattice each edge belongs to only one triangle and each site belongs to two triangles, therefore one can combine first two summations in (3) and Hamiltonian for kagome lattice can be written in the following form:

$$H = \sum_{Triangles} \left[ \frac{J_2 - J_3}{2} (\boldsymbol{\sigma}_i \boldsymbol{\sigma}_j + \boldsymbol{\sigma}_j \boldsymbol{\sigma}_k + \boldsymbol{\sigma}_k \boldsymbol{\sigma}_i) - \frac{\hbar}{2} (\sigma_i^z + \sigma_j^z + \sigma_k^z) \right]. \quad (6)$$

According to [6] the effective value of the exchange parameters  $J = J_2 - 2J_3$  on triangular lattice, which has been estimated experimentally from susceptibility and

specific-heat data for solid  $^3\text{He}$  is  $J = -3.07\text{mK}$ . Therefore, the three-site exchange ( $J_3$ ) is dominant on the triangular lattice. This is a consequence of the fact that on triangular lattice, for high densities the probability of a triple permutations of  $^3\text{He}$  atoms is dominant than a pair one. In the case of fluid  $^3\text{He}$ , which is described by kagome lattice, pair exchanges become more probable, since every edge belongs to one triangle and one hexagon, in contrast to the triangular lattice for which every edge belongs to two triangles. Moreover, we did not take into account the six-site exchange interaction which is the antiferromagnetic one. Taking into account above mentioned facts we can consider effective pair exchange permutations ( $J_2$ ) more dominant than three-site one ( $J_3$ ).

### 3 Basic Gibbs-Bogoliubov mean-field formalism

Here we apply the variational mean-field like treatment based on Gibbs-Bogoliubov inequality [25] to solve the Hamiltonian (6). This implies that the free energy (Helmholtz potential) of system is

$$F \leq F_0 + \langle H - H_0 \rangle_0, \quad (7)$$

where  $H$  is the real Hamiltonian which describes the system and  $H_0$  is the trial one.  $F$  and  $F_0$  are free energies corresponding to  $H$  and  $H_0$  respectively and  $\langle \dots \rangle_0$  denotes the thermal average over the ensemble defined by  $H_0$ . By introducing trial Hamiltonian for our model (Eq. (6) kagome lattice) containing unknown variational parameters one can minimize right hand side of Bogoliubov inequality (7) and get the values of those parameters,

For antiferromagnetic interactions, the trial Hamiltonian will consist of two parts describing the two sublattices. We introduce a trial Hamiltonian  $H_0$  as a set of non-interacting clusters (triangles) on two sublattices in different external self-consistent fields:

$$H_0 = \sum_{\Delta_i} H_0^{(i)}, \quad (8)$$

where

$$H_0^{(i)} = \lambda \times (\sigma_1^i \sigma_2^i + \sigma_2^i \sigma_3^i + \sigma_3^i \sigma_1^i) - \gamma_v \times [(\sigma_1^i)^z + (\sigma_2^i)^z + (\sigma_3^i)^z], \quad (9)$$

where  $\lambda$  and  $\gamma_v$  variational parameters, and  $\Delta_i$  labels different noninteracting rectangles (see Fig. 1, grey triangles) and

$$\begin{aligned} \gamma_v &= \gamma_a && \text{for sublattice (a),} \\ \gamma_v &= \gamma_b && \text{for sublattice (b).} \end{aligned} \quad (10)$$

It should be emphasized that in trial Hamiltonian spins  $\sigma_k^i$  of the  $\Delta_i$ -th triangle do not interact with the spins  $\sigma_k^j$  of the  $\Delta_j$  triangle if  $i \neq j$ , therefore these spins are

statistically independent. Suppose the real Hamiltonian  $H$  (6) can be represented in the following form

$$H = \sum_{\Delta_i} H^{(i)}, \quad (11)$$

where  $H^{(i)}$  is the contribution of spins on the single triangle in real Hamiltonian  $H$  and index of summation  $\Delta_i$  runs over the different triangles (see Fig. 1, grey triangles). Terms of real Hamiltonian  $\sigma_1^i \sigma_2^i + \sigma_2^i \sigma_3^i + \sigma_3^i \sigma_1^i$  must be included in  $H^{(i)}$ , but terms like  $\sigma_\alpha^i \sigma_\beta^j$  (see Fig. 1 solid lines) should be included both in  $H^{(i)}$  and  $H^{(j)}$ . Consequently,  $H^{(i)}$  has the following form:

$$H^{(i)} = \frac{J_2 - J_3}{2} \left( \alpha^{(i)} + \sum_{\tau=2,3} \frac{\sigma_1^i \sigma_\tau^j}{2} + \sum_{k=1,3} \frac{\sigma_2^i \sigma_\tau^k}{2} + \sum_{a=1,2} \frac{\sigma_3^i \sigma_\tau^l}{2} \right) - h \sum_{\tau=1}^3 (\sigma_\tau^i)^z, \quad (12)$$

where

$$\alpha^{(i)} = \sigma_1^i \sigma_2^i + \sigma_2^i \sigma_3^i + \sigma_3^i \sigma_1^i. \quad (13)$$

In the expressions for  $H^{(i)}$  we take half of each term  $\sigma_a^i \sigma_b^j$  because this term should be included in two different triangles.

Inequality (7) can be rewritten now for the single triangle on each sublattice ( $v$ ):

$$f_v \leq (f_0)_v + \langle H^{(i)} - H_0^{(i)} \rangle_0, \quad (14)$$

where  $H^{(i)}$  is the real and  $H_0^{(i)}$  the trial Hamiltonians of the triangle,  $f_v$  and  $(f_0)_v$  free energies of the one triangle on sublattice ( $v$ ) defined by  $H^{(i)}$  and  $H_0^{(i)}$  respectively. By denoting magnetizations of the sublattices ( $a$ ) and ( $b$ ) respectively  $m_a$  and  $m_b$  and taking into account that spins  $\sigma_\tau^i$  belong to sublattice ( $a$ ) and spins  $\sigma_\tau^{j,k}$  belong to sublattice ( $b$ ) and fact that spins  $\sigma_\tau^i$  and  $\sigma_\tau^{j,k}$  ( $i \neq j, k$ ) are statistically independent we get:  $\langle (\sigma_\tau^i)^{x,y} \rangle = 0$ ,  $m_a \equiv \langle (\sigma_\tau^i)^z \rangle / 2$ ,  $m_b \equiv \langle (\sigma_\tau^{j,k})^z \rangle / 2$  and  $\langle \sigma_\tau^i \sigma_\tau^j \rangle = \langle (\sigma_a^i)^z \rangle \times \langle (\sigma_b^j)^z \rangle = 2m_a 2m_b$ . One can rewrite inequality (14) as follows:

$$f_v \leq (f_0)_v + \left( \frac{J_2 - J_3}{2} - \lambda \right) \langle \alpha \rangle_0 + \frac{J_2 - J_3}{4} 6(2m_a 2m_b) - (h - \gamma_v) 6m_v.$$

$$\gamma_a = h - (J_2 - J_3)m_b, \quad \gamma_b = h - (J_2 - J_3)m_a.$$

Minimizing the right hand side of (15) in order to  $\gamma_a, \gamma_b$  and  $\lambda$  and using the fact, that  $\frac{\partial f_0}{\partial \lambda} = \langle \alpha \rangle_0$  and  $\frac{\partial f_0}{\partial \gamma_v} = -6m_v$  we obtain the following values for the variational parameters:

$$\begin{aligned} \lambda &= \frac{J_2 - J_3}{2}, \\ \gamma_a &= h - (J_2 - J_3)m_b, \\ \gamma_b &= h - (J_2 - J_3)m_a. \end{aligned} \quad (15)$$

The Hamiltonian  $H_0^{(i)}$  was chosen to be exactly solved. By diagonalization Hamiltonian  $H_0^{(i)}$  one can find eigenvectors and eigenvalues of the trial Hamiltonian [21, 27].

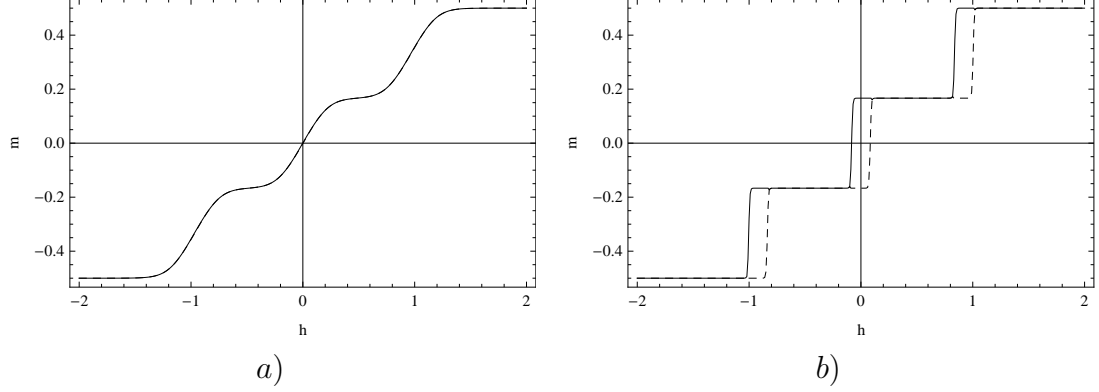


Figure 2: Magnetization  $m_a$  versus external magnetic field  $h$  for  $J_2 = 3 \text{ mK}$ ,  $J_3 = 2.5 \text{ mK}$ . at a)  $T=0.15 \text{ mK}$  b)  $T=0.01 \text{ mK}$ .

## 4 Magnetic properties

Here and further exchange parameters ( $J_2, J_3$ ) and magnetic field  $h$  is taking in Boltzman's constant scaling i.e. Boltzmann's constant is set to be  $k_B = 1$ .

The results of the previous section can be used for investigation of the magnetic properties of our model. The magnetization of arbitrary site is defined as

$$m_v = \frac{\text{Tr}(S_v e^{-H/T})}{Z} \quad (16)$$

$S_v$  corresponding spin operator on sublattice ( $v$ ),  $H$  is the Hamiltonian (9) with constants (15) and  $Z$  is partition function of the system. But according to (15) the Hamiltonian of sublattice ( $a$ ) depends on  $m_b$  through  $\gamma_a$  and vice versa. For defined above magnetization we obtain the following expression:

$$m_a = \frac{1}{6} \cdot \frac{3 \sinh\left(\frac{3\gamma_a}{T}\right) + \sinh\left(\frac{\gamma_a}{T}\right) + 2e^{\left(\frac{6\lambda}{T}\right)} \sinh\left(\frac{\gamma_a}{T}\right)}{\cosh\left(\frac{3\gamma_a}{T}\right) + \cosh\left(\frac{\gamma_a}{T}\right) + 2e^{\left(\frac{6\lambda}{T}\right)} \cosh\left(\frac{\gamma_a}{T}\right)}, \text{ and } \gamma_a = h - (J_2 - J_3)m_b. \quad (17)$$

The dependance of magnetization  $m_a$  from external magnetic field  $h$  can be found by solving the this recursive equation for each value of magnetic field  $h$ .

At relatively high temperatures the recursive equation has one stable solution and therefore magnetization curves of sublattices ( $a$ ) and ( $b$ ) coincide (see Fig. 2(a)). With decreasing temperature the solution of recursive equation ceases to be stable and, therefore, the magnetization of different sublattices are no longer equal. The partially saturated phase emerges in form of the magnetization plateaus (see Fig. 2(b) for  $T = 0.01 \text{ mK}$ ,  $J_2 = 3 \text{ mK}$ ,  $J_3 = 2.5 \text{ mK}$ ), which can be associated with a staggered magnetization or short range antiferromagnetism (AF) in frustrated kagome geometry. Indeed, the appearance of plateaus in magnetization curve at  $m = \pm 1/6$  can be explained as stability of trimeric states in available ( $\uparrow\uparrow\downarrow, \uparrow\downarrow\uparrow, \downarrow\uparrow\uparrow$ ) and ( $\uparrow\downarrow\downarrow, \downarrow\uparrow\downarrow, \uparrow\downarrow\downarrow$ ) configurations. Moreover, zero field magnetisation of one sublattice

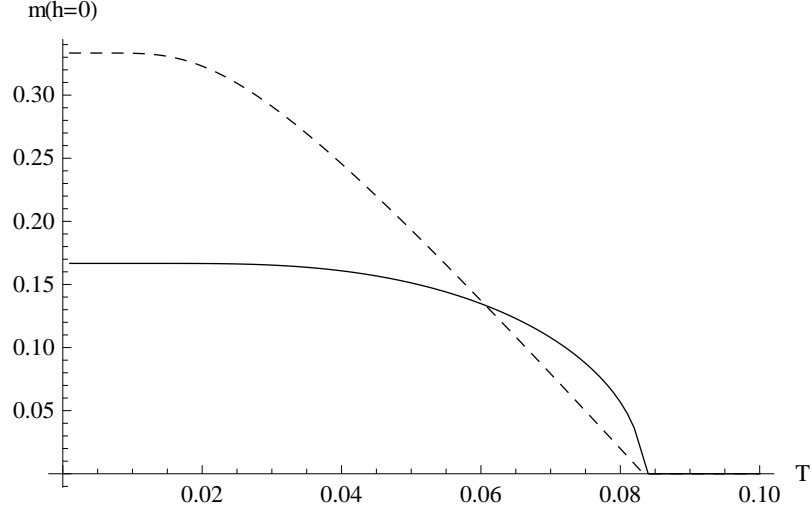


Figure 3: Dependence of the magnetization  $m_a$  (solid line) and concurrence (dashed line) at zero external field from temperature  $T$  at  $J_2 = 3$  mK,  $J_3 = 2.5$  mK.

becomes nonzero. In figure 3 the solid line shows the temperature dependence of the magnetization in the absence of external magnetic field. The magnetization tends gradually to zero near the second-order transition temperature  $T_C$  between ordered  $m_a \neq 0$  and disordered  $m_a = 0$  phases.

## 5 Concurrence and thermal entanglement

The mean-field like treatment transforms kagome lattice to the set of noninteracting triangles in effective field, therefore quantum correlations can be exactly accounted. This allows in terms of three-qubit XXX Heisenberg model in effective magnetic field  $\gamma$  to study the thermal entanglement properties. We will study the concurrence as a measure of pairwise entanglement [24]. The concurrence  $C(\rho)$  corresponding to the density matrix  $\rho$  is defined as

$$C(\rho) = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}, \quad (18)$$

where  $\lambda_i$  are the square roots of the eigenvalues of the operator

$$\tilde{\rho} = \rho_{12}(\sigma_1^y \otimes \sigma_2^y)\rho_{12}^*(\sigma_1^y \otimes \sigma_2^y), \quad (19)$$

where  $\rho_{12} = \text{Tr}_3 \rho$  is the reduced density matrix of the pair and  $\rho$  is defined in the following way

$$\rho = \frac{1}{Z} \sum_{i=1}^8 e^{-\frac{E_i}{T}} |\psi_i\rangle \langle \psi_i|, \quad (20)$$

where  $Z$  is the partition function of the system and  $\psi_i$  and  $E_i$  are eigenvectors and eigenvalues of the Hamiltonian  $H_0^{(i)}$  respectively (see Eq. 9).  $\rho_{12}$  has the following

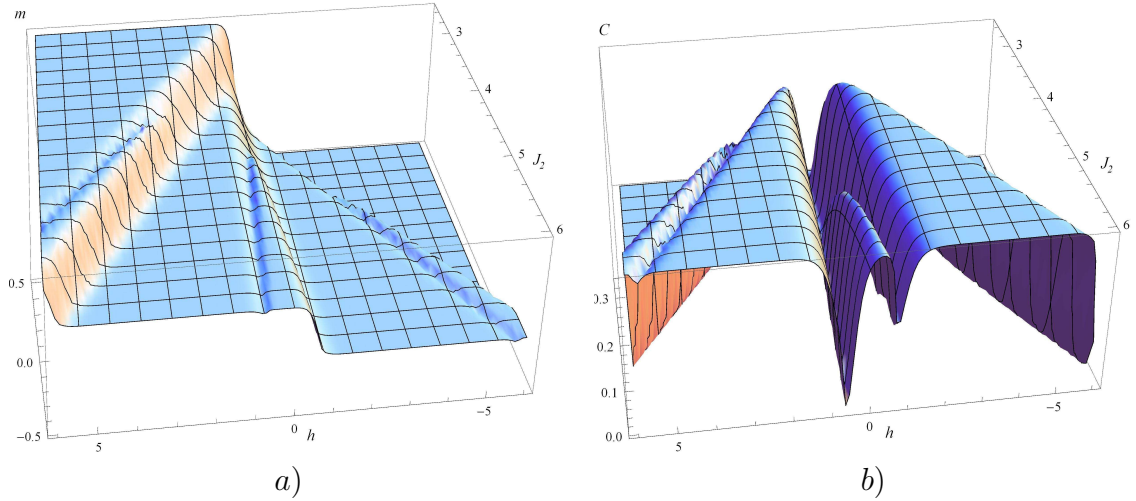


Figure 4: Dependence for (a) magnetization  $m$  and (b) concurrence  $C(\rho)$  versus the magnetic field  $h$  and the coupling constant  $J_2$  at  $J_3 = 2.5 \text{ mK}$  and  $T = 0.2 \text{ mK}$ .

form

$$\rho_{12} = \begin{pmatrix} u & 0 & 0 & 0 \\ 0 & w & y & 0 \\ 0 & y & w & 0 \\ 0 & 0 & 0 & v \end{pmatrix}, \quad (21)$$

where  $u, w, y$  and  $v$  are some functions of variables  $\gamma, \lambda$  and  $T$ . Using (18), (19) and (21) one can find the following expression for the concurrence  $C(\rho)$

$$C(\rho) = \max\{|y| - \sqrt{uv}, 0\}. \quad (22)$$

In this equation one must replace  $\gamma$  with  $h - 2(J_2 - J_3)m$  (see Eq.(15)), therefore the concurrence  $C(\rho)$  is the function of magnetisation  $m$ . To calculate concurrence one must solve transcendental equation (17) for each set of parameter values  $(J_2, J_3, h, T)$  and insert corresponding solution to the equation (22).

It is curious to discuss some similarities of statistical and quantum characteristics of our system. We consider magnetization as a statistical characteristic. In figure 3(a) plotted the magnetization as a function of the coupling constant  $J_2$  (for fixed value of  $J_3 = 2.5 \text{ mK}$ ) and the external field  $h$ , at a relatively high temperature  $T = 0.2 \text{ mK}$ . As a quantum characteristic we consider entanglement (concurrence  $C(\rho)$ ). In figure 3(b) the concurrence as a function of the  $J_2$  ( $J_3 = 2.5 \text{ mK}$ ) is shown for the same value of temperature. Our calculations show that the magnetic characteristics is similar to that of bipartite entanglement. Indeed, comparison of figures 3(a) and 3(b) shows that regions corresponding to the magnetization plateaus, coincide with the plateaus on concurrence plot.



## 6 Conclusion

In this paper we find strong correlations between magnetic properties and quantum entanglement in the Heisenberg model with two-, and three-site exchange interactions in strong magnetic field on the kagome lattice, which correspond to the third layer of fluid  $^3\text{He}$  absorbed on the surface of graphite. We adopted variational mean-field-like treatment (based on the Gibbs-Bogoliubov inequality) of separate clusters in effective magnetic fields and studied magnetic properties and concurrence as a measure of pairwise thermal entanglement. The system exhibits different magnetic behaviors, depending on the values of the exchange parameters ( $J_2, J_3$ ). We have obtained the magnetization plateaus at low temperatures. We have found, that in the antiferromagnetic region behavior of the concurrence coincides with the magnetization one. The comparison of magnetization and concurrence shows that regions corresponding to the magnetization plateaus, coincide with the plateaus on concurrence plot.

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